

both treatments and controls, the ratio of basidiomycetes to ascomycetes changed significantly in response to litter removal, from a ratio of 12:1 of basidiomycete to ascomycete EM to a ratio of 3:1.

Together, these results indicate that these disturbances can cause changes in the EM fungal community. Because different species may perform different functions, these results

indicate that it is now necessary to assess changes to pivotal ecosystem functions. Thus, the next step of this study will be to perform assessments of changes in enzyme systems that are responsible for controlling both nitrogen and carbon cycles in forest ecosystems.

Point of Contact: K. Cullings
(650) 604-2773
kcullings@mail.arc.nasa.gov

Structure and Functions of Protocells

Andrew Pohorille, Michael A. Wilson

This research studies the origin of cellular functions, with a long-term objective to explain how protocells performed functions essential for their survival and evolution utilizing only molecules that may have been available in the protobiological milieu. Simple models of several protocellular functions have been developed, and computer simulations have been carried out using molecular dynamics (MD) computer simulations. In MD simulations, Newton's equations of motion are solved for all the atoms in the system under study, providing a complete time history of the system. Properties of interest are computed from the trajectory using classical statistical mechanics.

Probably the first cell-like structures were vesicles—closed, spheroidal assemblies of organic material enclosing an aqueous medium. The walls of vesicles are built of amphiphilic molecules that have water-soluble (hydrophilic) and water-insoluble (hydrophobic) groups at opposite ends. These molecules are arranged in bilayers such that the hydrophilic head groups point toward water and the hydrophobic tails form the interior of the bilayer. In this respect, vesicle walls resemble modern cell membranes. Under proper conditions, vesicles form spontaneously from an

aqueous solution of amphiphiles. Vesicles became the precursors to true cells—protocells—by acquiring the capabilities needed to survive and reproduce. Protocells had to transport ions and organic matter from the environment across their walls, capture and utilize energy, and synthesize the molecules necessary for self-maintenance and growth. The identity of molecules that performed these functions is open to debate. Because most metabolic functions in modern organisms are carried out by proteins, the most parsimonious assumption is that their protobiological precursors were peptides. Their protocellular potential is illuminated by the fact that a wide range of simple, naturally occurring or synthetic peptides can spontaneously insert into membranes and assemble into channels capable of transporting material across cell walls.

The stability of monomers and dimers of a peptide consisting of leucine (L) and serine (S) in a heptad repeat arrangement of (LSLLLLSL)₃ has been investigated in a membrane-like system consisting of an octane layer between two water layers. Both the transmembrane and parallel, in-plane orientations of the monomer correspond to stable states, with the parallel orientation being more stable. However, conversion between the two requires crossing a

large free energy barrier and a substantial structural rearrangement of the water molecules on both sides of the membrane.

Although a transmembrane dimer was found to be stable, a dimer oriented parallel to the interface was found to be unstable. This finding implies that the predominant state of an equilibrium distribution of peptides is a monomer parallel to the interface. Under the application of an external electric field, the monomers rotate into the transmembrane orientation, where they can aggregate into dimers and tetramers. Experiments in other laboratories have demonstrated that tetramers can function as channels for transporting protons across the membrane.

One goal of this research project is to construct multimeric, transmembrane structures that can function as primitive catalysts. In the present case, the peptide does not possess interactions that are specific enough to maintain a rigid structure that could contain a catalytic site because the transmembrane dimer structure, as shown in the figure, is much less rigid than a coiled-coil structure. It has been observed more generally that transmembrane proteins are not simply "inside-out" analogues of water-soluble proteins. Consequently, specific residues must be modified to achieve the packing that is typical of water-soluble coiled coils.

Point of Contact: A. Pohorille
(650) 604-5759
pohorill@raphael.arc.nasa.gov

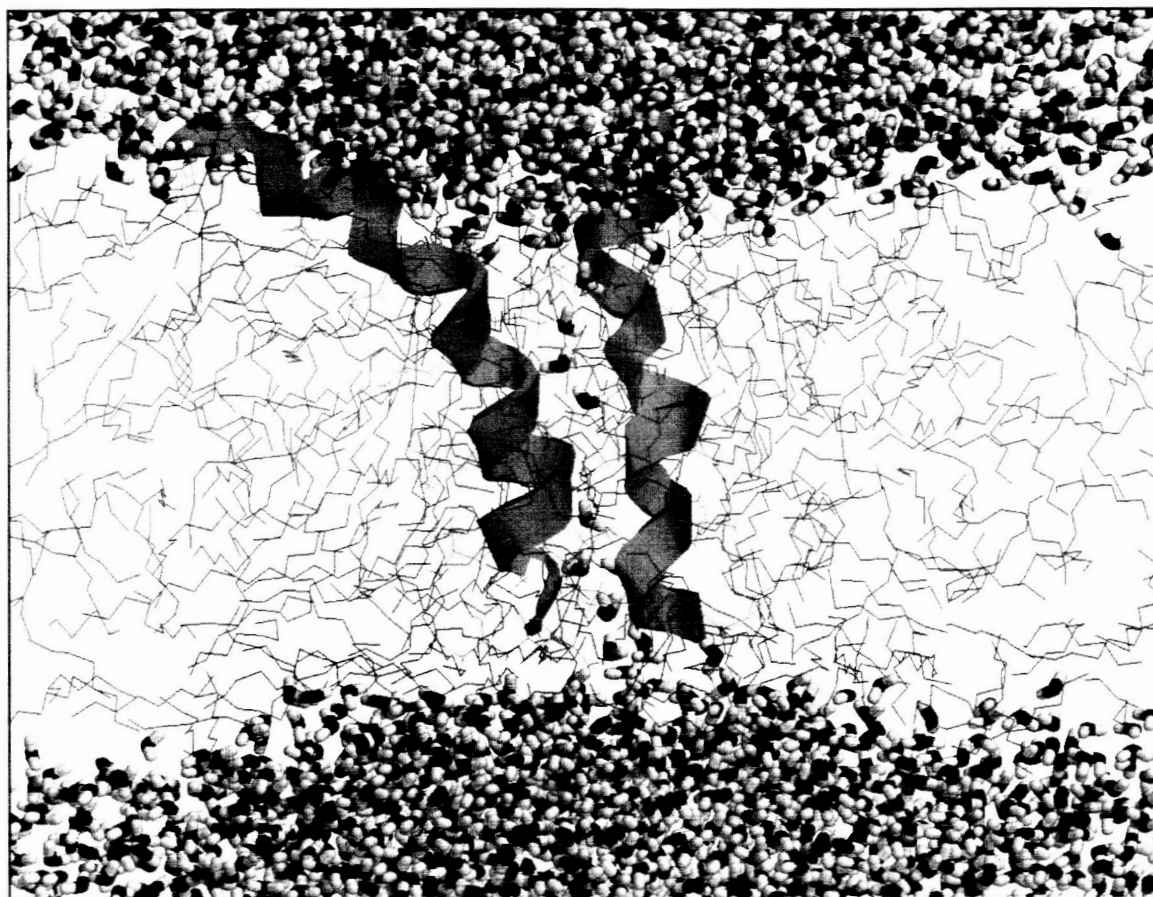


Fig. 1. Transmembrane dimer of $(LSLLSL)_3$. The peptide molecules are shown as gray helices, the octane is green, and the water is red and white. The disorder is evidenced by the separation of the helices and the significant water penetration into the membrane interior.